Computational Science: Modeling and Simulation

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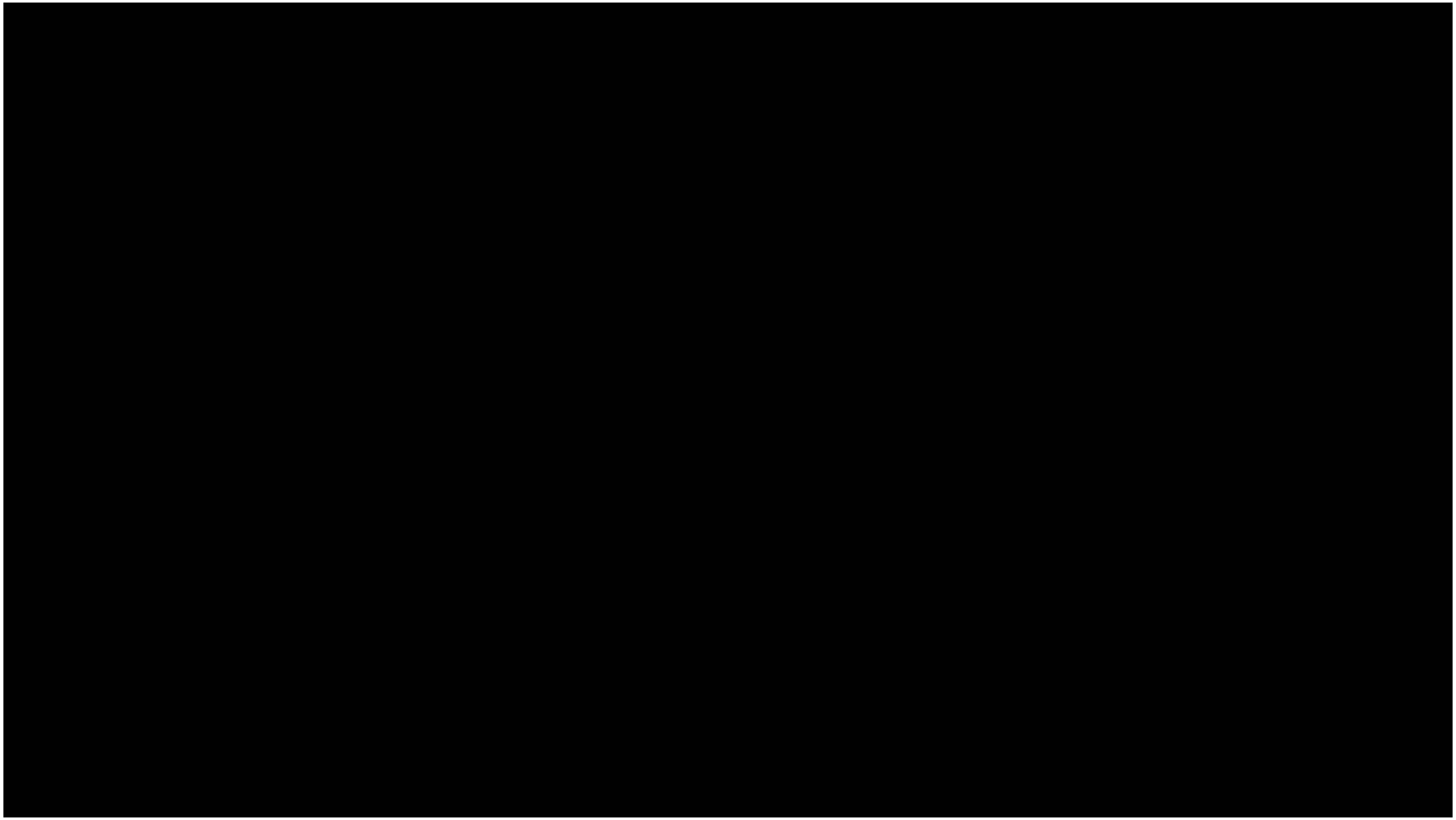


OSCILLATORY MOTIONS

Simple Harmonic Motion

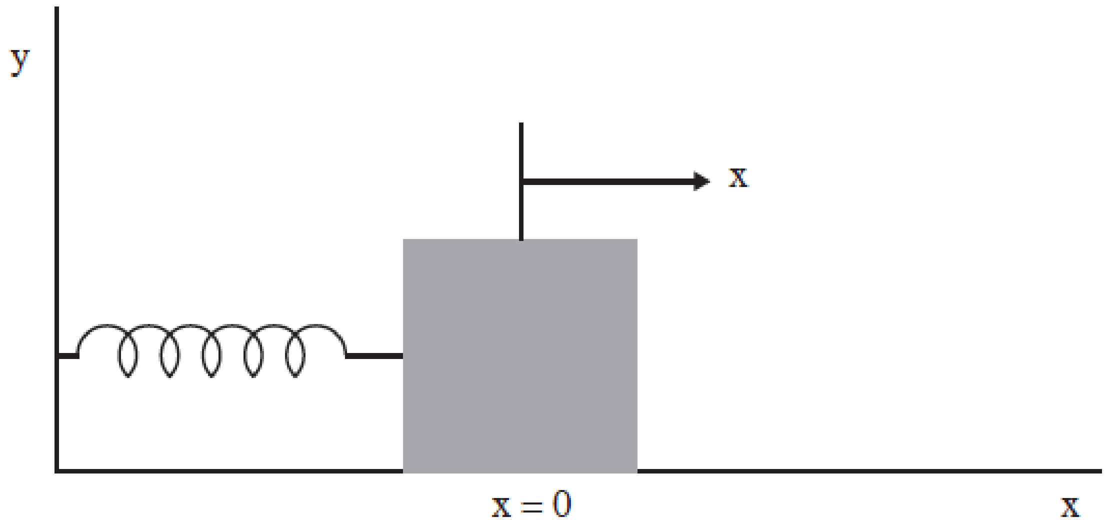


Figure 4.1: A one-dimensional harmonic oscillator. The block slides horizontally on the frictionless surface.

Simple Harmonic Motion

$$F = -kx.$$

$$\frac{d^2x}{dt^2} = -{\omega_0}^2 x,$$

the angular frequency ω_0 is defined by

$$ {\omega_0}^2 = \frac{k}{m}.$$

Amplitude

$$x(t) = A\cos(\omega_0 t + \delta),$$

Phase

Simple Harmonic Motion

$$x(t+T) = x(t).$$

Period T

$$T = \frac{2\pi}{\omega_0} = \frac{2\pi}{\sqrt{k/m}}.$$

The frequency ν of the motion is the number of cycles per second and is given by $\nu = 1/T$.

Simple Harmonic Motion

Although the position and velocity of the oscillator are continuously changing, the total energy E remains constant and is given by

Kinectic energy

$$E = \frac{1}{2}mv^2 + \frac{1}{2}kx^2 = \frac{1}{2}kA^2.$$

Total Energy

Potential energy

Problem 4.1. Energy conservation

a. Use the Euler `ODESolver` to solve the dynamical equations for a simple harmonic oscillator by extending `AbstractSimulation` and implementing the `doStep` method. (See Section 4.2 for an example of such a program for the pendulum.) Have your program plot $\Delta E_n = E_n - E_0$, where E_0 is the initial energy and E_n is the total energy at time $t_n = t_0 + n\Delta t$. (It is necessary only to consider the energy per unit mass.) Plot the difference ΔE_n as a function of t_n for several cycles for a given value of Δt. Choose $x(t = 0) = 1$, $v(t = 0) = 0$ and ${\omega_0}^2 = k/m = 9$ and start with $\Delta t = 0.05$. Is the difference ΔE_n uniformly small throughout the cycle? Does ΔE_n drift, that is, become bigger with time? What is the optimum choice of Δt?

b. Implement the Euler-Cromer algorithm by writing an Euler-Cromer ODESolver and answer the same questions as in part (a).

c. Modify your program so that the Euler-Richardson or Verlet algorithms are used and answer the same questions as in part (a). (The Verlet algorithm is discussed in Appendix 3.)

Problem 4.4. Superposition of waves

a. Write a program to plot $A\sin(kx+\omega t)$ from $x = x_{\min}$ to $x = x_{\max}$ as a function of t. (Implement an `AbstractSimulation` rather than an `AbstractCalculation`.) For simplicity, take $A = 1$, $\omega = 2\pi$, and $k = 2\pi/\lambda$, and $\lambda = 2$.

b. Modify your program so that it plots the sum of $y_1 = \sin(kx - \omega t)$ and $y_2 = \sin(kx + \omega t)$. The quantity $y_1 + y_2$ corresponds to the superposition of two waves. Choose $\lambda = 2$ and $\omega = 2\pi$. What kind of a wave do you obtain?

c. Use your program to demonstrate beats by plotting $y_1 + y_2$ as a function of time in the range $x_{\min} = -10$ and $x_{\max} = 10$. Determine the beat frequency for each of the following superpositions: $y_1(x,t) = \sin[8.4(x - 1.1t)]$, $y_2(x,t) = \sin[8.0(x - 1.1t)]$; $y_1(x,t) = \sin[8.4(x - 1.2t)]$, $y_2(x,t) = \sin[8.0(x - 1.0t)]$; and $y_1(x,t) = \sin[8.4(x - 1.0t)]$, $y_2(x,t) = \sin[8.0(x - 1.2t)]$. What difference do you observe between these superpositions?

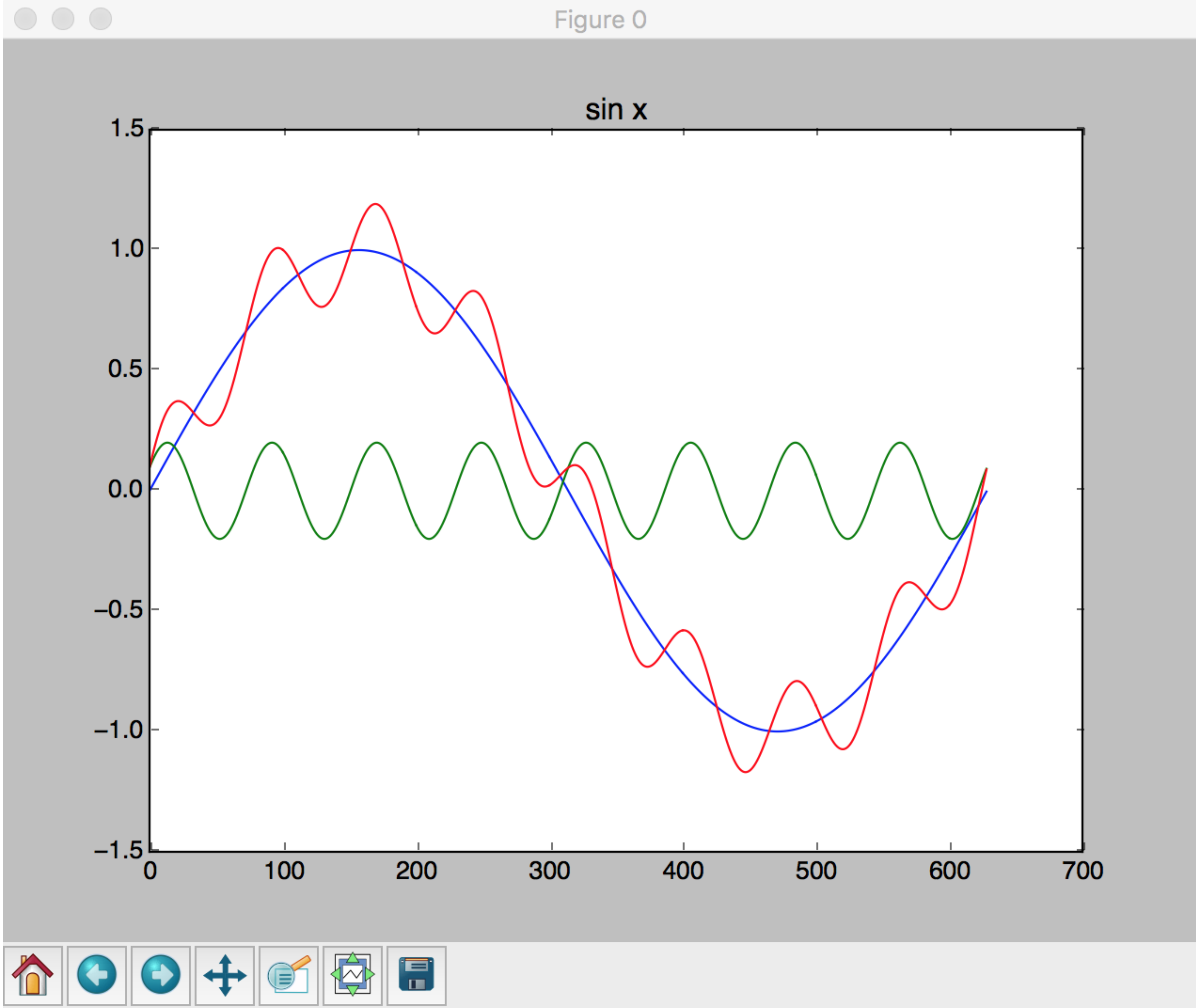
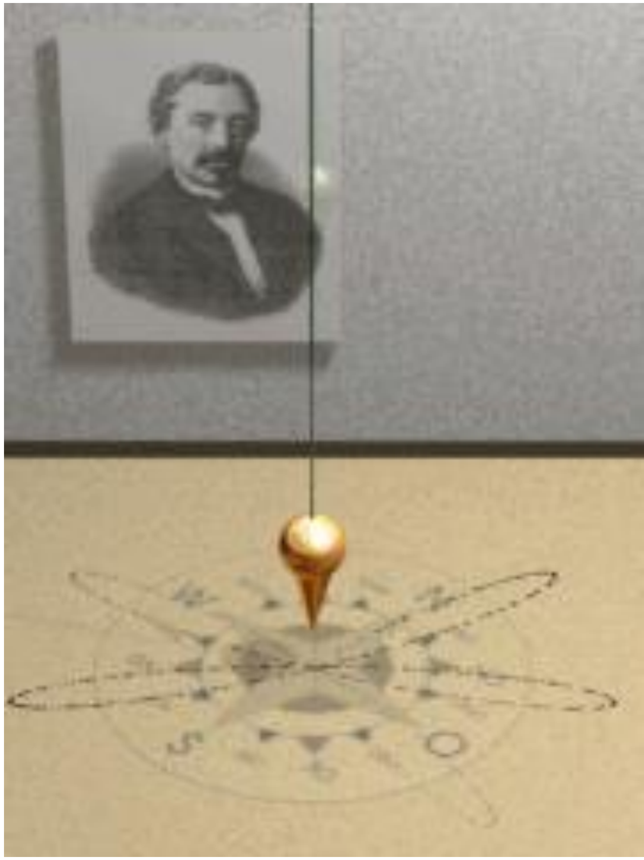


Figure 0
sin x
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
0
100
200
300
400
500
600
700

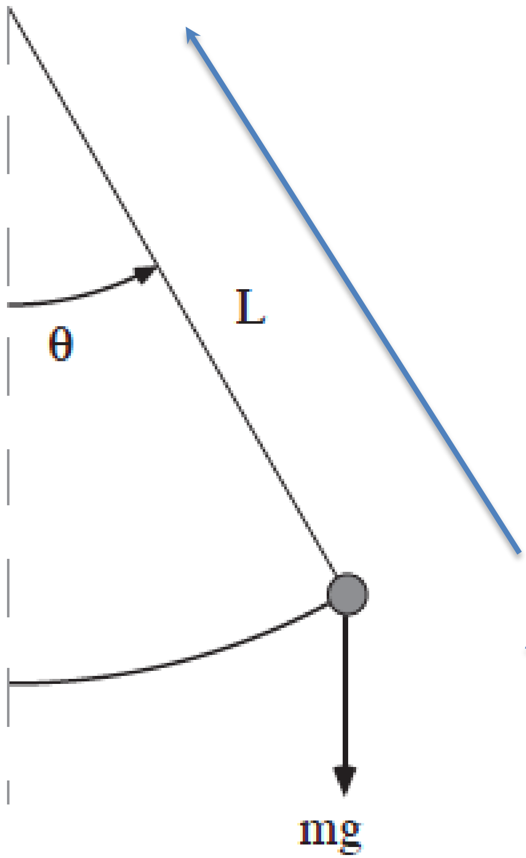
PENDULUM

Foucault Pendulum



Foucault Pendulum

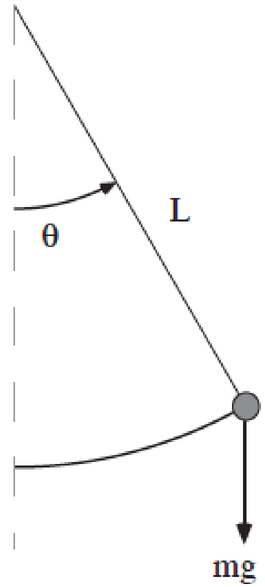
Pendulum



$$v = L\frac{d\theta}{dt}$$
$$a = L\frac{d^2\theta}{dt^2}.$$

Forces: g and rod L

Pendulum



$$v = L\frac{d\theta}{dt}$$

$$a = L\frac{d^2\theta}{dt^2}.$$

$$mL\frac{d^2\theta}{dt^2} = -mg\sin\theta,$$

$$\frac{d^2\theta}{dt^2} = -\frac{g}{L}\sin\theta.$$

Non-linear equations which seldom have simple analytical solutions

Pendulum

$$v = L\frac{d\theta}{dt}$$

$$a = L\frac{d^2\theta}{dt^2}.$$

$$mL\frac{d^2\theta}{dt^2} = -mg\sin\theta,$$

$$\frac{d^2\theta}{dt^2} = -\frac{g}{L}\sin\theta.$$

For small amplitudes: $\sin\theta \approx \theta,$

$$\frac{d^2\theta}{dt^2} \approx -\frac{g}{L}\theta. \qquad (\theta \ll 1)$$

Pendulum

Compare!

$$\frac{d^2x}{dt^2} = -{\omega_0}^2 x,$$

$$\frac{d^2\theta}{dt^2} \approx -\frac{g}{L}\theta. \qquad (\theta \ll 1)$$

$$T = 2\pi\sqrt{\frac{L}{g}}. \qquad \text{(small amplitude oscillations)}$$

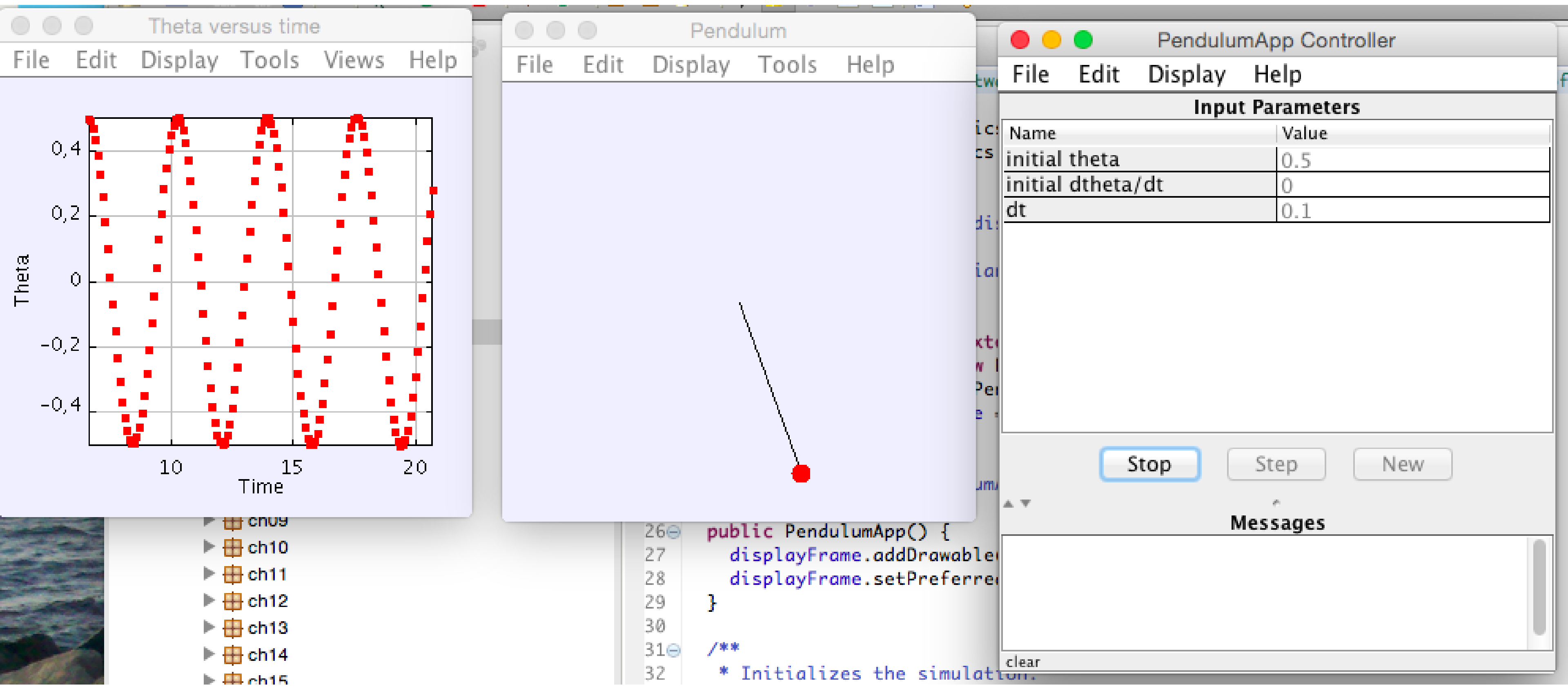
One way to understand the motion of a pendulum with large oscillations is to solve (4.11) numerically. Because we know that the numerical solutions must be consistent with conservation of energy, we derive the form of the total energy here. The potential energy can be found from the following considerations. If the rod is deflected by the angle θ, then the bob is raised by the distance $h = L - L\cos\theta$ (see Figure 4.2). Hence, the potential energy of the bob in the gravitational field of the earth is

$$U = mgh = mgL(1 - \cos\theta), \tag{4.14}$$

where the zero of the potential energy corresponds to $\theta = 0$. Because the kinetic energy of the pendulum is $\frac{1}{2}mv^2 = \frac{1}{2}mL^2(d\theta/dt)^2$, the total energy E of the pendulum is

$$E = \frac{1}{2}mL^2\left(\frac{d\theta}{dt}\right)^2 + mgL(1 - \cos\theta). \tag{4.15}$$

pendulumApp



Damped Harmonic Oscillator

Damped coefficient

$$\frac{d^2x}{dt^2} = -{\omega_0}^2 x - \gamma \frac{dx}{dt}.$$

Problem 4.6. Damped linear oscillator

a. Incorporate the effects of damping into your harmonic oscillator simulation and plot the time dependence of the position and the velocity. Describe the qualitative behavior of $x(t)$ and $v(t)$ for $\omega_0 = 3$ and $\gamma = 0.5$ with $x(t = 0) = 1$, $v(t = 0) = 0$.

b. The period of the motion is the time between successive maxima of $x(t)$. Compute the period and corresponding angular frequency and compare their values to the undamped case. Is the period longer or shorter? Make additional runs for $\gamma = 1$, 2, and 3. Does the period increase or decrease with greater damping? Why?

c. The amplitude is the maximum value of x during one cycle. Compute the *relaxation time* τ, the time it takes for the amplitude of an oscillation to decrease by $1/e \approx 0.37$ from its maximum value. Is the value of τ constant throughout the motion? Compute τ for the values of γ considered in part (b) and discuss the qualitative dependence of τ on γ.

d. Plot the total energy as a function of time for the values of γ considered in part (b). If the decrease in energy is not monotonic, explain.

e. Compute the time dependence of $x(t)$ and $v(t)$ for $\gamma = 4$, 5, 6, 7, and 8. Is the motion oscillatory for all γ? How can you characterize the decay? For fixed ω_0, the oscillator is said to be *critically damped* at the smallest value of γ for which the decay to equilibrium is monotonic. For what value of γ does critical damping occur for $\omega_0 = 4$ and $\omega_0 = 2$? For each value of ω_0, compute the value of γ for which the system approaches equilibrium most quickly.

Response to External Forces

$$\frac{d^2x}{dt^2} = -{\omega_0}^2 x - \gamma v + \frac{1}{m}F(t).$$

$$\frac{1}{m}F(t) = A_0 \cos \omega t,$$

External force

Problem 4.8. Response of a driven damped linear oscillator

a. Modify your simple harmonic oscillator program so that an external force of the form (4.18) is included. Add this force to the class that encapsulates the equations of motion without changing the target class. The angular frequency of the driving force should be added as an input parameter.

b. Choose $\omega_0 = 3$, $\gamma = 0.5$, $\omega = 2$ and the amplitude of the external force $A_0 = 1$ for all runs unless otherwise stated. For these values of ω_0 and γ, the dynamical behavior in the absence of an external force corresponds to an underdamped oscillator. Plot $x(t)$ versus t in the presence of the external force with the initial condition, $x(t = 0) = 1, v(t = 0) = 0$. How does the qualitative behavior of $x(t)$ differ from the nonperturbed case? What is the period and angular frequency of $x(t)$ after several oscillations? Repeat the same observations for $x(t)$ with $x(t = 0) = 0, v(t = 0) = 1$. Identify a transient part of $x(t)$ that depends on the initial conditions and decays in time, and a steady state part that dominates at longer times and is independent of the initial conditions.

ELECTRIC CIRCUIT OSCILLATIONS

element	voltage drop	symbol	units
resistor	$V_{\mathrm{R}} = IR$	resistance R	ohms (Ω)
capacitor	$V_{\mathrm{C}} = Q/C$	capacitance C	farads (F)
inductor	$V_{\mathrm{L}} = L\,dI/dt$	inductance L	henries (H)

Table 4.1: The voltage drops across the basic electrical circuit elements. Q is the charge (coulombs) on one plate of the capacitor, and I is the current (amperes).

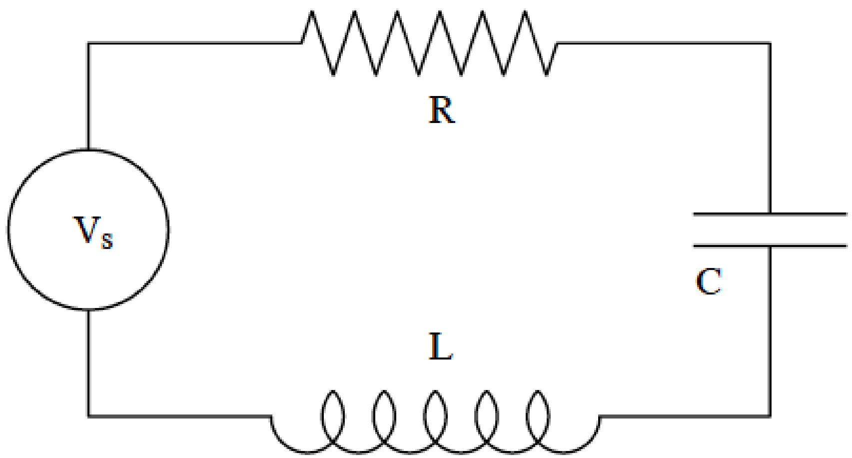


Figure 4.5: A simple series RLC circuit with a voltage source V_s.

$$V_{\mathrm{L}} + V_{\mathrm{R}} + V_{\mathrm{C}} = V_s(t).$$

$$I = dQ/dt.$$

$$L\frac{d^2Q}{dt^2} + R\frac{dQ}{dt} + \frac{Q}{C} = V_s(t),$$

Electric circuit	Mechanical system
charge Q	displacement x
current $I = dQ/dt$	velocity $v = dx/dt$
voltage drop	force
inductance L	mass m
inverse capacitance $1/C$	spring constant k
resistance R	damping γ

Table 4.2: Analogies between electrical parameters and mechanical parameters.

RC model

$$L\frac{d^2Q}{dt^2} + R\frac{dQ}{dt} + \frac{Q}{C} = V_s(t),$$

$$\frac{d^2x}{dt^2} = -{\omega_0}^2 x - \gamma v + \frac{1}{m}F(t).$$

Damped Harmonic Oscillator with External Force

Exercício: implemente o modelo abaixo usando Euler.

$$L\frac{d^2Q}{dt^2} + R\frac{dQ}{dt} + \frac{Q}{C} = V_s(t),$$

Electric circuit	Mechanical system
charge Q	displacement x
current $I = dQ/dt$	velocity $v = dx/dt$
voltage drop	force
inductance L	mass m
inverse capacitance $1/C$	spring constant k
resistance R	damping γ

Table 4.2: Analogies between electrical parameters and mechanical parameters.

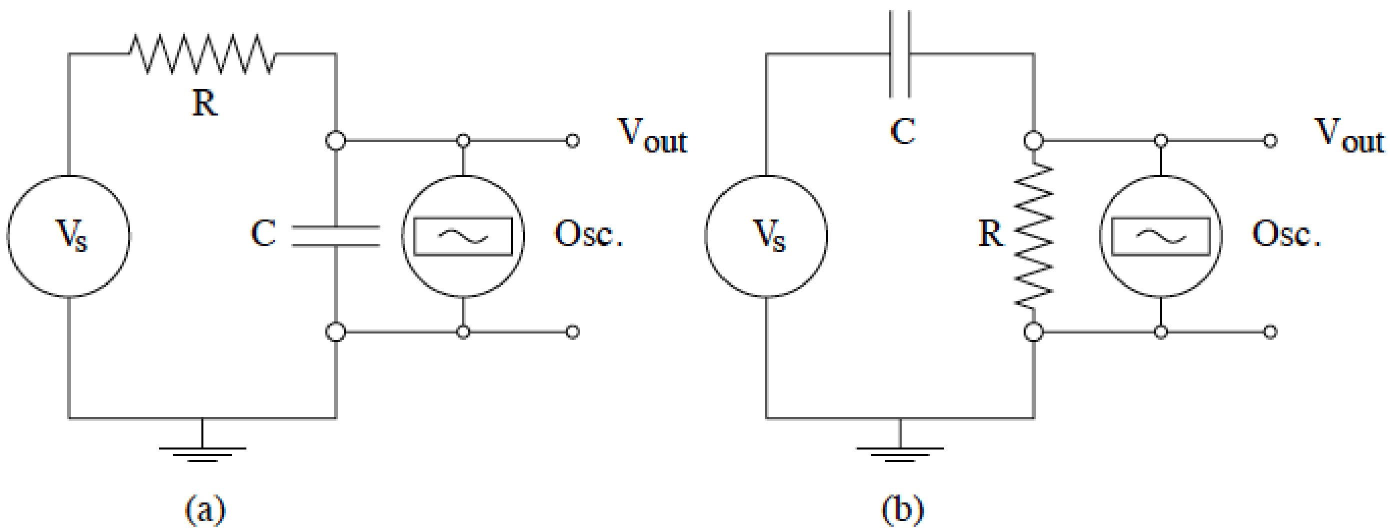
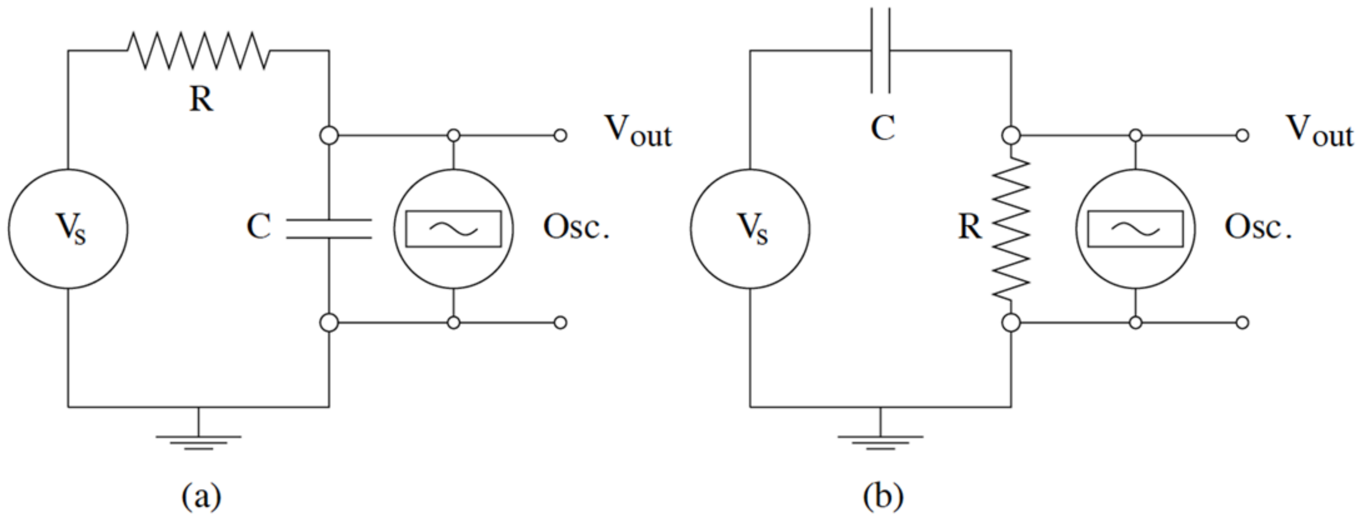


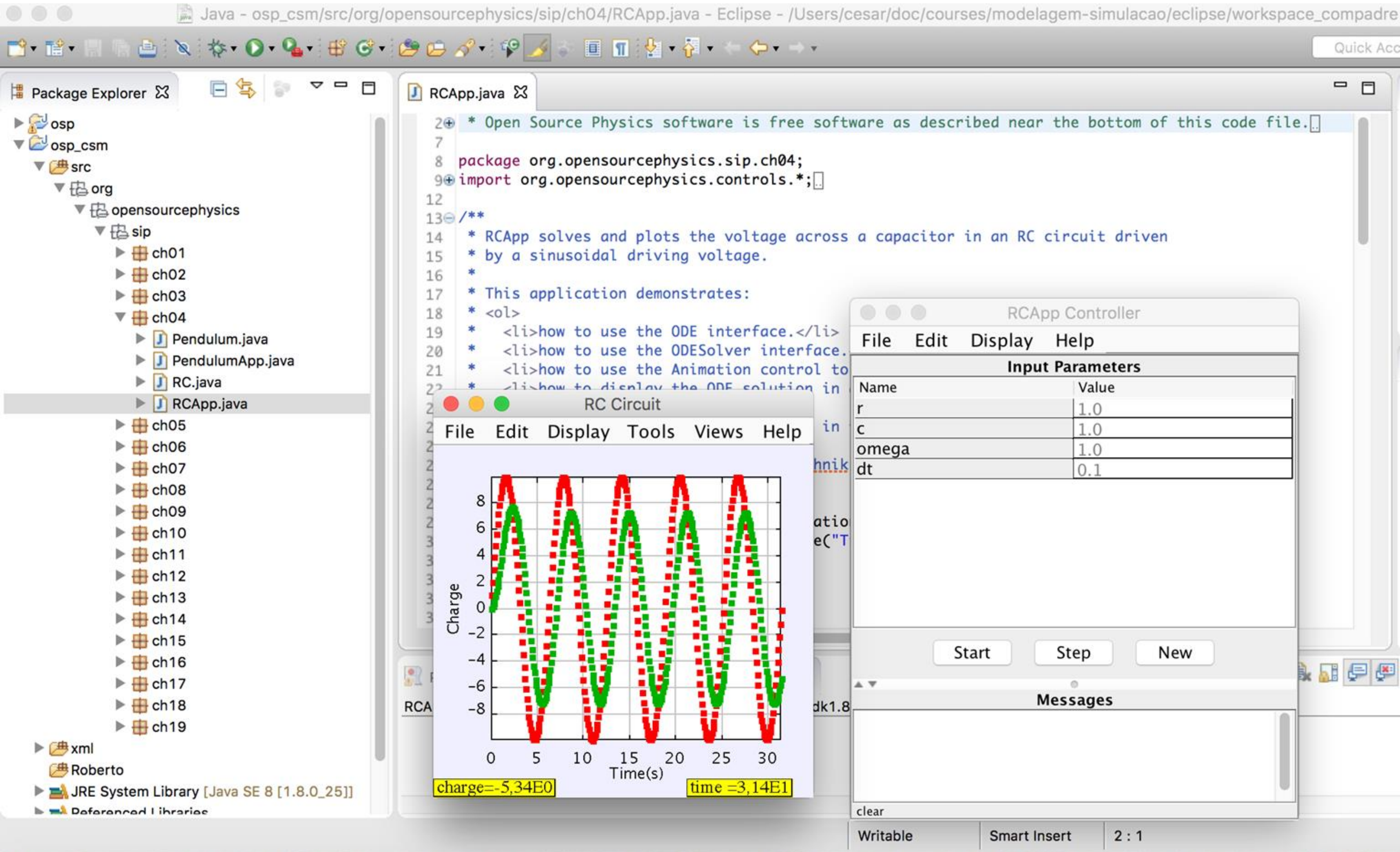
Figure 4.6: Examples of RC circuits used as low and high pass filters. Which circuit is which?



$$RI(t) = R\frac{dQ}{dt} = V_s(t) - \frac{Q}{C}.$$

```java
  /**
   * Get the source voltage at given time.
   * @param t
   * @return
   */
  public double getSourceVoltage(double t) {
    return 10*Math.sin(omega*t);
  }

  /**
   * Get the rate array. Implementation of ODE interface.
   * This method may be invoked many times with different intermediate states
   * as an ODESolver is carrying out the solution.
   *
   * @param state the state array
   * @param rate the rate array
   */
  public void getRate(double[] state, double[] rate) {
    rate[0] = (-state[0]/r/c)+(getSourceVoltage(state[1])/r); // dQ/dt
    rate[1] = 1;                                              // dt/dt = 1
  }
}
```


Java - osp_csm/src/org/opensourcephysics/sip/ch04/RCApp.java - Eclipse - /Users/cesar/doc/courses/modelagem-simulacao/eclipse/workspace_compadre
Package Explorer
osp
osp_csm
src
org
opensourcephysics
sip
ch01
ch02
ch03
ch04
Pendulum.java
PendulumApp.java
RC.java
RCApp.java
ch05
ch06
ch07
ch08
ch09
ch10
ch11
ch12
ch13
ch14
ch15
ch16
ch17
ch18
ch19
xml
Roberto
JRE System Library [Java SE 8 [1.8.0_25]]
RCApp.java
* Open Source Physics software is free software as described near the bottom of this code file.
package org.opensourcephysics.sip.ch04;
import org.opensourcephysics.controls.*;
/**
* RCApp solves and plots the voltage across a capacitor in an RC circuit driven
* by a sinusoidal driving voltage.
*
* This application demonstrates:
*
* how to use the ODE interface.
* how to use the ODESolver interface.
* how to use the Animation control to
RC Circuit
File Edit Display Tools Views Help
Charge
Time(s)
charge=-5,34E0
time =3,14E1
RCApp Controller
File Edit Display Help
Input Parameters
Name Value
r 1.0
c 1.0
omega 1.0
dt 0.1
Start Step New
Messages
clear
Writable Smart Insert 2 : 1

4.6 Accuracy and Stability

Project 4.18. Nerve impulses

In 1952 Hodgkin and Huxley developed a model of nerve impulses to understand the nerve membrane potential of a giant squid nerve cell. The equations they developed are known as the Hodgkin-Huxley equations. The idea is that a membrane can be treated as a capacitor where $CV = q$ and thus the time rate of change of the membrane potential V is proportional to the current, dq/dt, flowing through the membrane. This current is due to the pumping of sodium and potassium ions through the membrane, a leakage current, and an external current stimulus. The model is capable of producing single nerve impulses, trains of nerve impulses, and other effects. The model is described by the following first-order differential equations:

$$C\frac{dV}{dt} = -g_K n^4(V - V_K) - g_{Na}m^3h(V - V_{Na}) - g_L(V - V_L) + I_{\text{ext}}(t) \tag{4.30a}$$

$$\frac{dn}{dt} = \alpha_n(1 - n) - \beta_n n \tag{4.30b}$$

$$\frac{dm}{dt} = \alpha_m(1 - m) - \beta_m m \tag{4.30c}$$

$$\frac{dh}{dt} = \alpha_h(1 - h) - \beta_h h, \tag{4.30d}$$

Material de trabalho

- Leia o Capítulo 4 do livro texto.
- Resolva os exercícios desse capítulo.
- Procure o monitor ou o professor para suas dúvidas.

Material extra para o futuro

Problem 4.12. Simple filter circuits

Problem 4.13. Square wave response of an RC circuit

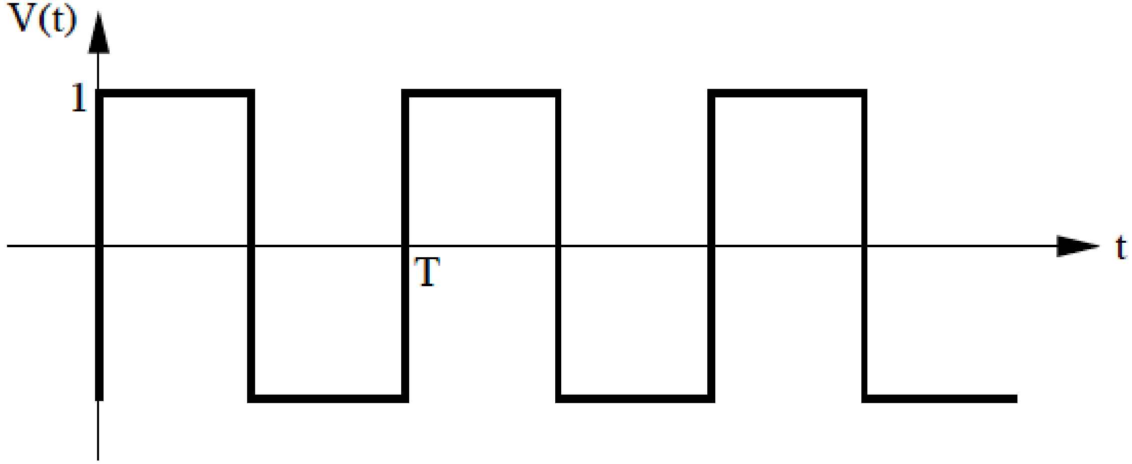


Figure 4.7: Square wave voltage with period T and unit amplitude.